Statistical mechanics of scale-free networks at a critical point: Complexity without irreversibility?

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Based on a rigorous extension of classical statistical mechanics to networks, we study a specific microscopic network Hamiltonian. The form of this Hamiltonian is derived from the assumption that individual nodes increase/decrease their utility by linking to nodes with a higher/lower degree than their own. We interpret utility as an equivalent to energy in physical systems and discuss the temperature dependence of the emerging networks. We observe the existence of a critical temperature T_c where total energy (utility) and network-architecture undergo radical changes. Along this topological transition we obtain scale-free networks with complex hierarchical topology. In contrast to models for scale-free networks introduced so far, the scale-free nature emerges within equilibrium, with a clearly defined microcanonical ensemble and the principle of detailed balance strictly fulfilled. This provides clear evidence that 'complex' networks may arise without irreversibility. The results presented here should find a wide variety of applications in socio-economic statistical systems.

Triggered by the vast number of observed non-trivial networks in nature, recently a respectable number of models have been introduced to understand their statistical properties. Since many of these networks differ considerably from pure random graphs [1], the notion of complex networks has emerged which is a nowadays well established concept [2, 3]. Perhaps the most apparent property distinguishing such 'complex' real-world networks from pure random graphs is their scale-free degree distribution $P(k) \sim k^{-\gamma}$, which seems to be ubiquitous in nature [3]. Further, many real-world networks exhibit a high amount of clustering, and sometimes even a non-trivial dependence of the clustering coefficient, C_i of node i, when seen as a function of its degree k_i. A power form of $\langle C(k)\rangle \sim k^{-\delta}$ can be associated to the 'complex' topological property of hierarchical clustering [4]. Allmost all of the microscopic models proposed to describe such 'complex', growing or static, networks involve non-equilibrium and evolutionary elements, manifesting themselves in different procedures of preferential attachment [5–8] or other structured rewirement schemes [9–11]. Further, these procedures often involve the need for non-local information. The reasoning behind these approaches has further solidified the notion of complex networks. The concept of non-equilibrium in the context of networks is so dominant, that recently even structured rewirement schemes have entered the very definition of network-ensembles [3, 12]. Less drastic views of ensembles of networks have recently been used to generalize random graphs to networks with arbitrary degree [13], and to generate scale-free networks by appropriately tuning the weights of 'network-Feynman graphs' [14].

So far, comparatively little has been done to understand complex networks from a purely classical statistical mechanics point of view, fully satisfying its foundations such as equal a-priori probabilities. Aiming at an explanation of scale-free networks based on microscopic interactions, several serious equilibrium approaches have been proposed [15–17]. In particular topological properties of networks associated with specific Hamiltonians have been studied [9, 16, 17]. The Hamiltonians investigated there lead to interesting dynamics, but – to our knowledge – not to scale-free, complex networks.

The aim of this paper is to close this fundamental gap by proposing a Hamiltonian leading to scale-free, hierarchic networks in thermal equilibrium. The form of the Hamiltonian is derived from simple, general, and socio-economically motivated assumptions about individual utilities of nodes. Nodes act as utility maximizers, such as physical particles minimize energy. For the greater ease of the exposition of our model we shall use the notions of utility and inverse energy interchangeably.

We consider symmetric networks with a fixed number of distinguishable nodes $i = 1, ..., N$, connected by a fixed number of $\ell = 1, ..., L$ indistinguishable links. The network is represented by its adjacency matrix $\mathbf{c}$, where $c_{ij} = c_{ji} = 1$, if a link connects nodes i and j and $c_{ij} = c_{ji} = 0$, otherwise. Thus, we define the microcanonical partition function as

$$\Omega(E, N, L) = \sum_{P(\mathbf{c})} \frac{1}{L!} \delta(E - \mathcal{H}(\mathbf{c}))\delta(L - \mathrm{Tr}(\frac{\mathbf{c}^2}{2})) , \quad (1)$$

with $\mathcal{H}(\mathbf{c})$ being the network Hamiltonian and $P(\mathbf{c})$ denoting all permutations of the $N \times N$ adjacency-matrix. This definition guarantees that each possible configuration of the adjacency matrix is realized with the same a priori probability. The canonical partition function may be obtained by the Laplace transform of Eq. (1), [18], or via the maximum entropy principle, as shown in [16],

$$Z(T, N, L) = \sum_{P(\mathbf{c})} \delta\left(L - \frac{Tr(\mathbf{c}^2)}{2}\right) e^{-\beta\mathcal{H}(\mathbf{c})} , \quad (2)$$

using the usual definition of temperature $T \equiv \frac{1}{k\beta}$. In

simulations the canonical ensemble can be generated e.g. by the Metropolis-algorithm: starting from an adjacency matrix $\mathbf{c}$, a 'virtual' graph $\hat{\mathbf{c}}$ is generated by a random rewirement step. Then, $\hat{\mathbf{c}}$ is accepted with probability $p_{accept} = \min(1, \exp[-\beta(\mathcal{H}(\hat{\mathbf{c}}) - \mathcal{H}(\mathbf{c}))])$.

Given Eq. (2) one may study any reasonable Hamiltonian depending on any properties of the network. Here, we want to adopt the view of modeling *microscopic* interactions, where the total energy of a network can be expressed as the sum over all energy/utility contributions of individual nodes, u_i. In many realistic settings this node-utility will depend on properties/states of node i itself, and on properties of the node j whereto a link is established. These node-properties are denoted by $\Pi(i)$. In this case the Hamiltonian is also expressible as a sum over all links,

$$\mathcal{H}(\mathbf{c}) = \sum_{\ell=1}^{L} u_\ell(\Pi(i), \Pi(j)) , \quad (3)$$

where $u_\ell(\Pi(i), \Pi(j))$ is the utility of link ℓ connecting nodes i and j, who are characterized by their properties $\Pi(i)$ and $\Pi(j)$, respectively. For simplicity we assume linearity and separate u_ℓ into the individual node-contributions $u_\ell(\Pi(i), \Pi(j)) = u_i(\Pi(i), \Pi(j)) + u_j(\Pi(i), \Pi(j))$. In the following we specify the model such that the utility of a node increases if it connects to a node that is 'more important' than itself. Similarly, its utility decreases if it establishes a (potentially costly) link to a 'less important' node. As a simple measure for importance we suggest the degree of a node, i.e. $\Pi(i) = k_i$. The relative importance between two nodes is denoted by $\Delta k = |k_i - k_j|$, which will enter the utility function as the only argument. For the particular form of the utility function we chose a standard, monotonically increasing, concave log-utility function [19], which incor-

porates the concept of decreasing marginal utility [19]. We thus model node-utility by

$$u_i(k_i, k_j) = \begin{cases} c_1 + a_1 \log(b_1 + \Delta k) & \text{for } k_i > k_j \\ c_2 - a_2 \log(b_2 + \Delta k) & \text{for } k_i < k_j \end{cases} \quad (4)$$

with shape parameters a and b, and offsets c. To avoid discontinuity in the utility function we set $c_2 = c_1 + a_1 \log(b_1) + a_2 \log(b_2)$. This function is shown in Fig. 1. For the sake of further simplicity, we assume $b_1 = b_2 = b$, to obtain a particularly simple form for the link-utility,

$$u_\ell(k_i, k_j) = c_1 + c_2 + (a_1 - a_2) \log(b + \Delta k) . \quad (5)$$

Parameter c_1 can be chosen to ensure positive total utility for each link. Parameter b controls the curvature of the utility function [19], and will be called 'sensitivity parameter' in the following.

Equation (5) can be interpreted as the inverse energy of each link which allows us to perform simulations of the associated canonical ensemble, Eq. (2). The (collective) amount of 'irrationality' of individual nodes, i.e. that nodes do not fully maximize their utility (by error or ignorance) is captured by the 'temperature' T. For $a_1 = a_2$, the utility is independent of Δk and we obtain random networks, as expected. For $a_1 \neq a_2$, the constants a and c can be absorbed in the temperature scale (Boltzmann constant) of the system; hence they are omitted without loss of generality. We assume that $a_1 > a_2$, meaning that the concave utility-contribution of lower degree is more dominant than the convex utility-contribution from the node of larger degree, (putting more emphasis on wins than on losses) leading to an asymmetry in utility, Fig. 1. We finally base our simulations on the Hamiltonian,

$$\mathcal{H}(\mathbf{c}) = -\sum_\ell \log(b + \Delta k) . \quad (6)$$
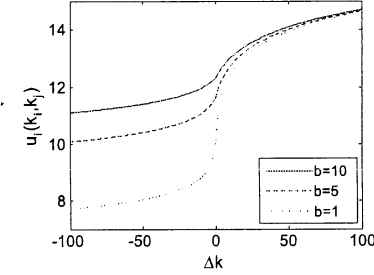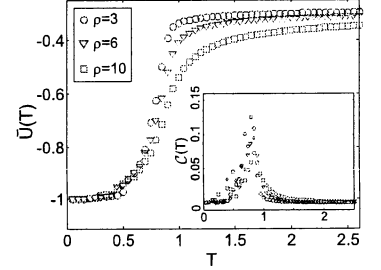

FIG. 1: Node-utility as a function of $\Delta k = k_i - k_j$ for different values of b. The parameters in Eq. (4) are $a_1 = 1$, $c_1 = 10$, $a_2 = 0.5$ and $c_2 = 1.5$.

FIG. 2: Ensemble average of normalized internal energy $\bar{U}(T) = U(T)/\min(U(T))$ and specific heat $\mathcal{C}(T)$ (inset) as a function of T, for $N = 10^3$, $b = 5$ and various densities ρ.
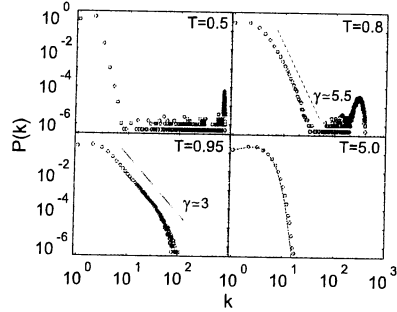
FIG. 3: Degree distributions at different temperatures for $N = 10^3$, $\rho = 3$, and $b = 5$. The line for $T = 5$ is the Poissonian $p(k) = \frac{e^{-\rho}\rho^k}{k!}$.

Based on Eq. (6) we simulate networks of the canonical ensemble, Eq. (2), ranging from $N = 500$ to 10^4 nodes. For computational reasons, temperature-dependent results are presented for $N = 10^3$. All ensemble-averages have been calculated from at least 2×10^3 configurations, separated by at least $20 \times N$ update steps. We analyze the obtained networks as a function of the model parameters – temperature (irrationality) T, link density $\rho = 2L/N$ and the 'sensitivity' parameter b.

Figure 2 shows the ensemble average of the total energy of the system as a function of T for different values of ρ. For better comparison data has been normalized to the minimum energy. Also shown is the specific heat C, obtained by a numeric derivative of the energy-data. One clearly finds a radical change in the energy and a characteristic maximum of the specific heat at about $T_c = 0.8 - 0.85$, indicating the presence of a critical point. The transition softens for higher link-densities, as well as for lower values of b (not shown). We refrain from commenting on the size of the underlying critical exponents, whose proper extraction is beyond the scope of this work.

The change in energy is associated with considerable restructuring of the underlying networks. To discuss this in more detail we have calculated ensemble-averages of degree distributions for various points along the transition. The results are shown in Fig. 3 for $N = 10^3$, $\rho = 3$ and $b = 5$. For temperatures up to about $T \sim 0.5$, we observe networks with degrees of all magnitudes. From $T \sim 0.5$ upward, a core of highly connected nodes (bump) keeps growing, gradually shifting to the left. For $T \lesssim 0.8$, the two regions in the degree distribution coexist. In the interval $0.8 \lesssim T \lesssim 0.95$, the highly connected core merges with the rest of the network and gradually disappears
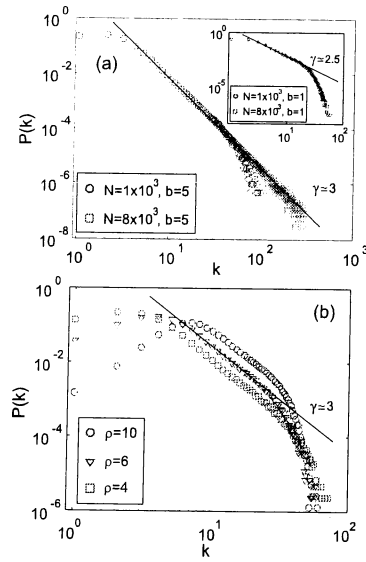

FIG. 4: (a) Finite size dependence of the degree distribution for various N and b (inset) and $\rho = 3$. For $b = 5$, we have $T = 0.95$, being somewhat higher for $b = 1$. (b) Degree distribution for different link-densities ρ, $N = 10^3$, and $b = 5$. Temperatures are adjusted to the pure scale-free region.

with further temperature increase. At $T \sim 0.95$ a pure power-law $P(k) \sim k^{-\gamma}$ with exponent $\gamma \sim 3$ matches the degree distribution. Ignoring the bump at higher degrees, the degree distribution may also be approximated reliably for lower temperatures (down to about $T \sim 0.80$). In the T interval $[0.80, 0.95]$ the degree exponent covers a range of $\gamma \in [5.5, 3]$, respectively. Increasing the temperature above $T = 0.95$, keeps the power-law exponent γ practically unchanged, but shifts the exponential cutoff to the left, ultimately leading to random networks with Poissonian distributions, Fig. 3.

Finite-size effects and the role of parameter b for the scale-free region are captured in Fig. 4 a. Sizes $N = 10^3$ and $N = 8 \times 10^3$ are compared for $b = 1$ and $b = 5$; both exhibit nice scaling. Power-law fits yield a degree exponent of $\gamma \approx 3$ and 2.5 for $b = 5$ and $b = 1$, respectively, regardless of system size. Variation of b therefor allows to model virtually all exponents occurring in real-world
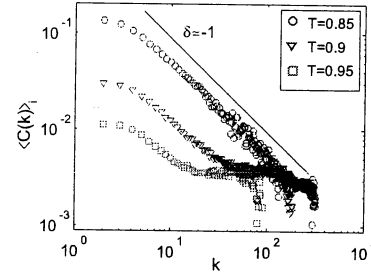
FIG. 5: Degree-dependence of the average cluster coefficient $\langle C(k) \rangle$ at different temperatures. $N = 10^3$, $\rho = 3$ and $b = 5$.

networks [3].

In Fig. 5 we show the degree-dependence of ensemble averages of the mean cluster coefficient $\langle C_i \rangle_i = \langle 2n_i/k_i(k_i - 1) \rangle_i$ where n_i is the number of links between the neighbors of node i, [20]. For $T = 0.85$ we obtain a nice scaling-law $\langle C(k) \rangle = k^\delta$, with $\delta = -1$. This is in very good agreement with many empirically examined data [4] and demonstrates that our model reproduces the 'complex' topological property of hierarchical clustering found in many socio-economical networks. For higher temperatures, δ stays the same, however, the onset of the cutoff regime changes, resulting in a flat curve for high temperatures (not shown).

The results presented hold qualitatively for relatively small ρ. For ρ larger than 5, a characteristic scale gradually emerges, due to the fact that the mean $\langle k \rangle$, corresponding to high-temperature random networks, shifts to larger values. Despite this characteristic scale, for appropriate temperatures, a power-law may still be fitted to a region, Fig. 4 b. Here temperatures are chosen such that the pure scale-free region is recovered (without the bump). The characteristic exponent of $\gamma = 3$ is preserved.

In summary, in the course of a very general modeling of socio-economical systems, where individuals are utility maximizers with bounded rationality, we discovered that scale-free networks with hierarchical clustering naturally emerge in the vicinity of a critical point. Most remarkably, the mechanism behind these results is nothing but the theory of equilibrium statistical mechanics, rigorously applied to networks. In substantial contrast to work conducted earlier [9, 12], no modifications of the sampling of phase-space are used (clearly defined microcanonical ensemble) such that the full power of equilib-

rium statistical mechanics is retained. We have obtained the first reversible, equilibrium access to scale-free networks based on microscopic interactions satisfying detailed balance. Preferential attachment and structured rewirement schemes model many non-equilibrium processes in the real world adequately, however, it has to be noted that scale-free networks also exist within a pure equilibrium concept. Finally, as the notion of complexity is usually tightly connected to dissipative structures far from equilibrium, our results could stimulate a discussion about the actual complexity of 'complex' networks.

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[1] P. Erdös, A. Rényi, Publ. Math. Debrecen 6, 290 (1959); Publ. Math. Inst. Hung. Acad. Sci. 5, 17 (1960).
[2] A.-L. Barabasi, Rev. Mod. Phys. 74, 47 (2002).
[3] S. Dorogovtsev, J.F.F. Mendes, Evolution of Networks: From Biological Nets to the Internet and WWW, (Oxford University Press, 2003).
[4] E. Ravasz, A.-L. Barabasi, Phys. Rev. E 67, 026112 (2003).
[5] A.-L. Barabasi, R. Albert, Science 286, 509 (1999).
[6] M. Rosvall, K. Sneppen, Phys. Rev. Lett. 91, 178701 (2003).
[7] J.J. Ramasco, S.N. Dorogovtsev and R. Pastor-Satorras Phys. Rev. E 70, 036106 (2004).
[8] G. Caldarelli, A. Capocci, P. De Los Rios and M.A. Munoz, Phys. Rev. Lett. 89, 25 (2002).
[9] M. Baiesi, S.S. Manna, Phys. Rev. E 68, 047103 (2003).
[10] B.J. Kim, A. Trusina, P. Minnhagen and K. Sneppen, Eur. Phy. J. B 43, 369 (2005).
[11] S. Thurner, C. Tsallis, cond-mat/0506140.
[12] S.N. Dorogovtsev, J.F.F. Mendes and A.N. Samukhin, Nucl. Phys. B 666, 396 (2003).
[13] S. Abe, S. Thurner, cond-mat/0501429.
[14] Z. Burda, J.D. Correia and A. Krzywicki, Phys. Rev. E 64, 046118 (2001).
[15] J. Berg, M. Lässig, Phys. Rev. Lett. 89, 228701 (2002).
[16] J. Park, M.E.J. Newman, Phys. Rev. E 70, 066117 (2004).
[17] I. Farkas, I. Derenyi, G. Palla and T. Vicsek, Lect. Notes Phys. 650, 163 (2004); G. Palla, I. Derenyi, I. Farkas and T. Vicsek, Phys. Rev. E 69, 046117 (2004).
[18] W.T. Grandy, Foundations of Statistical Mechanics, (Kluwer Academic Publishers, 1987).
[19] J.E. Ingersoll, Theory of Financial Decision Making, (Rowman & Littlefield Publishers, 1987).
[20] Nimerical ensemble averages may lead to artifacts if $\langle C(k) \rangle$, in network realizations where the respective d egree k is not existing, are defined as $\langle C(k) \rangle = 0$.